Local Deformation Behavior of Metallic Polycrystals

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Unless special processing is used, most metallic materials are aggregate composites composed of single crystals. Each of these crystals is generally anisotropic in how it deforms both elastically and plastically. We are developing both the theoretical and numerical tools to allow us to probe the detailed local response of a variety of metallic polycrystals. The single crystal is represented by a model, which accounts for large deformation kinematics, anisotropic elasticity and thermal expansion, temperature and deformation rate sensitive plastic flow. This flow rule is based on mathematics used to represent thermally activated slip processes. The plastic hardening relationship used is based upon first order dislocation generation and annihilation processes. The rate of hardening is also a function of temperature and deformation rate. Plastic flow is restricted to occur only on prescribed slip systems. A polycrystal microstructural model has been developed which is based on a Voronoi tessellation growth process using statistical models for the spatial distribution of seed points. A particular microstructure composed of 48 individual crystals is given in Fig. 1, shown without intragranular subdivision.

The single-crystal model parameters were evaluated for tantalum and the model was applied to the microstructure given in Fig. 1. Each of the 48 crystals were assigned an initial crystallographic orientation chosen by random and given the ability to plastically deform on the twelve $\{110\}\langle111\rangle$ and twelve $\{112\}\langle111\rangle$ slip systems. The 2-D model was then deformed (quasi-static and isothermal at 23C) in plane-strain compression up to a true strain of 1.0. The top and bottom surfaces were frictionless with the bottom surface stationary. The left edge is prevented from displacing horizontally while the right surface is stress-free. Response of the model is given in Figs. 2 and 3. Although experiments have not yet been conducted to verify the accuracy of our representation of the local polycrystal deformation field, the vonMises stress results given in Fig. 2 suggest that this metal deforms in a highly heterogeneous manner. For the example shown, the vonMises stress values range between approximately 500 and 1100 MPa. The free surface on the right side of the sample also demonstrates significant inhomogeneity at this length scale. Surface roughening like this is observed experimentally. Interaction between grains also causes nonuniform deformation to occur within each crystal. All of these phenomena are due to the inherent anisotropic nature of metallic crystal deformation. These capabilities are being used to study the physics and statistics of the ductile deformation and damage process for a number of metallic materials.

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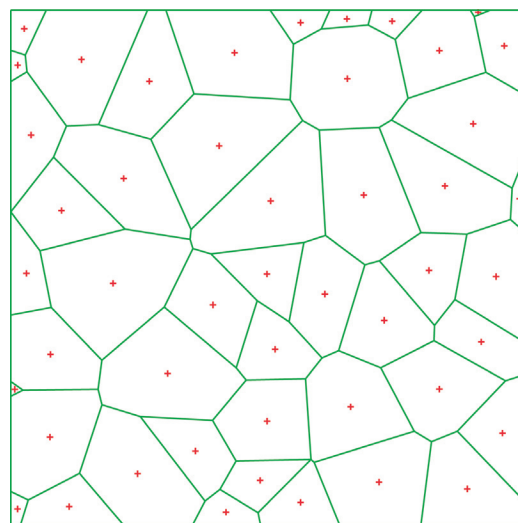
Fig. 1.
Voronoi tessellated microstructure (2-D) used for the plane-strain compression simulation. There are 48 grains in the aggregate polycrystal.
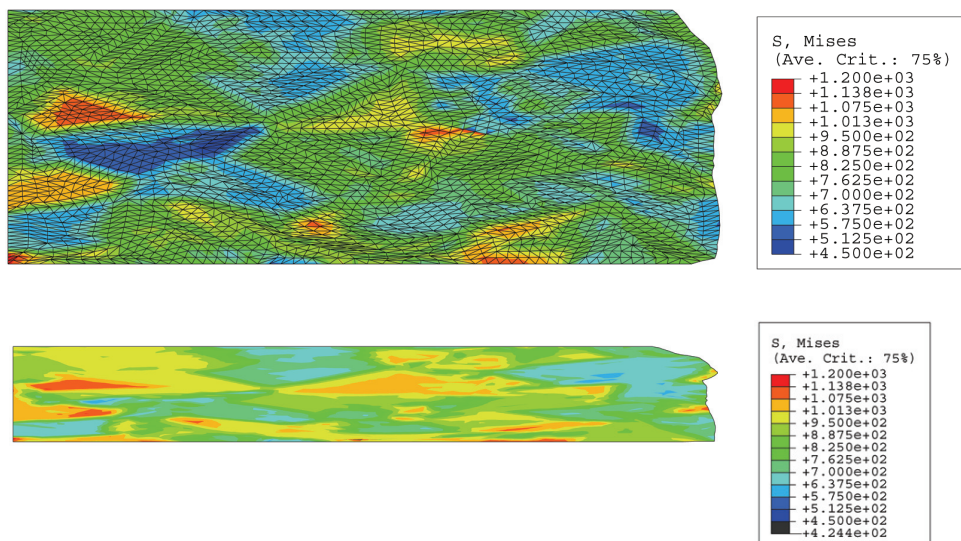
Fig. 2.
vonMises stress distribution within the tantalum polycrystal at a macroscopic compressive strain of (a) 0.52, with mesh shown; (b) 1.0, without mesh shown. The undeformed model is initially square.
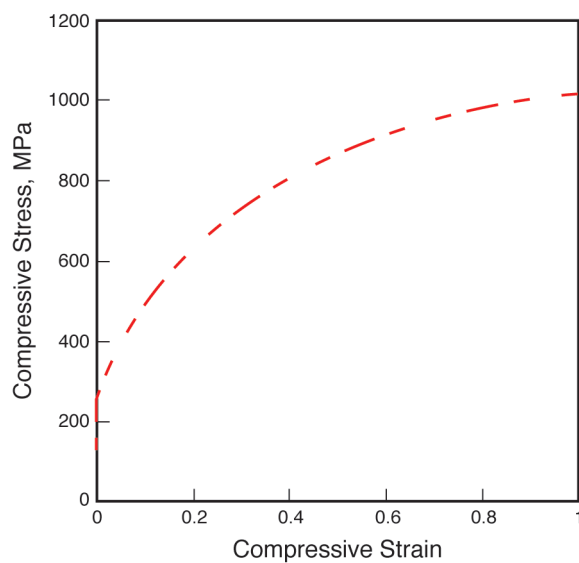
Fig. 3.
Macroscopic plane-strain compression stress-strain response for the 48-grain tantalum simulation.